LA-UR-19-24766
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Title: Mesoscale Connections Spring 2019

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Intended for: Newsletter
Web

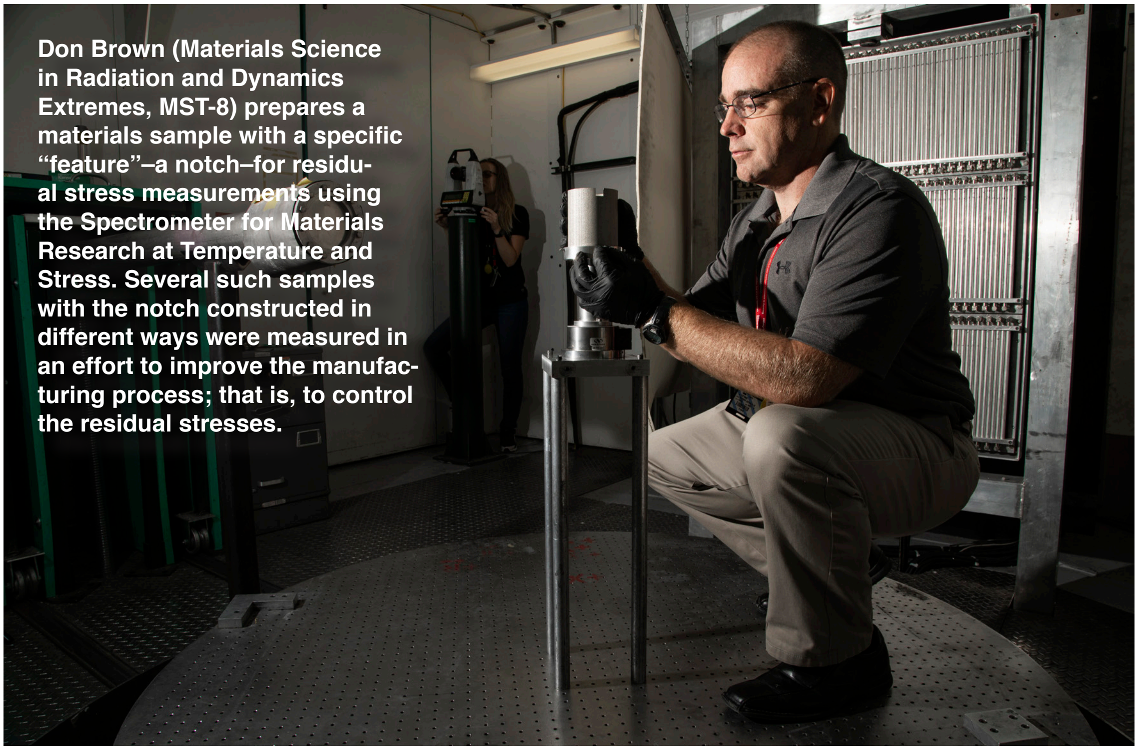
Issued: 2019-05-22

Spring 2019

Mesoscale Connections

Science and technology on the roadmap to DMMSC

INSIDE



Don Brown (Materials Science in Radiation and Dynamics Extremes, MST-8) prepares a materials sample with a specific "feature"–a notch–for residual stress measurements using the Spectrometer for Materials Research at Temperature and Stress. Several such samples with the notch constructed in different ways were measured in an effort to improve the manufacturing process; that is, to control the residual stresses.

Don Brown

Qualifying advanced manufacturing at the mesoscale with SMARTS

By H. Kris Fronzak, for ALDPS Communications

> *"Understanding the nation's existing stockpile isn't good enough. We are helping develop manufacturing processes that can create specific, controlled properties for a science-based qualification."*

Don Brown's latest mesoscale materials discovery is fresh from the SMARTS and HIPPO diffractometers at Los Alamos National Laboratory. Using this instrument suite, Brown and his team observed heat-treated manufactured metals to see the exact temperatures at which various material imperfections simply disappeared. This early investigation is one piece of a puzzle as Los Alamos researchers and their collaborators work to design advanced materials with specific performance to meet mission needs—a key objective of the Laboratory's Materials for the Future strategy.

As the leader of the Materials Science in Radiation and Dynamics Extremes' (MST-8) Scattering Science Team, Brown develops experiments and directs researchers using SMARTS (the Spectrometer for Materials Research at Temperature and Stress), and HIPPO (the High Pressure Preffered Orientation instrument). SMARTS and HIPPO rely on the Los Alamos Neutron Science Center's linear accelerator to propel neutrons that they can then direct through

continued on next page

Mesoscale Connections is published by the Physical Sciences Directorate. Its goal is to promote awareness of mesoscale materials research relevant to the NNSA, advances in mesoscale science capabilities at user facilities, and modeling challenges and needs for big data sets in service of materials co-design.

To read more about mesoscale materials science at Los Alamos National Laboratory, including past issues of this publication, visit www.lanl.gov/science-innovation/pillars/materials-science/mesoscale/index.php.

For information about the publication, please contact aldps-comm@lanl.gov.

*The **mesoscale** is the spatial scale that exists between atomic structures and the engineering continuum—critical to controlling macroscopic behaviors and properties.*

DMMSC is an experimental facility concept that could address an NNSA capability gap identified in a 2016 CD-0 for simultaneous characterization of microstructure and response at the mesoscale.

Formerly known as MaRIE, the Matter-Radiation Interactions in Extremes facility is Los Alamos's proposed solution that meets all the requirements of DMMSC. Our Mesoscale Materials Science program is developing capability and providing results on the road to the future.

National Nuclear Security Administration

Brown cont.

materials to determine atomic or magnetic structure. SMARTS can probe materials under the precise and often extreme conditions encountered in service, such as the 600 °C, high-pressure atmosphere needed for blades in jet engines or the extreme environment experienced by a missile. It can also identify weak points and stresses in bridge cables and can test parts as heavy as 3,300 lbs.

"Don specializes in local-scale probing of internal stress and dislocation structure. He's one of only a few individuals who is able to quantify what exists inside of a material," said colleague Curt Bronkhorst (Fluid Dynamics and Solid Mechanics, T-3). "The experiments he heads are critical for materials manufacturing and for the Lab's mission."

Brown and his teammates often probe at the mesoscale, a length scale that exists between the atomic and macro that is crucial to understanding materials' properties and controlling their performance. When coupled with the Lab's high-performance computing technology, the measuring abilities of SMARTS provide critical validation for advanced mesoscale models of materials.

"Understanding the nation's existing stockpile isn't good enough," said Brown. "We are helping develop manufacturing processes that can create specific, controlled properties for a science-based qualification."

One of the most complex challenges for SMARTS researchers is to modernize manufacturing methods to create metal parts with specific properties. By applying computational knowledge to advanced manufacturing techniques, Los Alamos scientists, working with data collected on SMARTS and HIPPO, can construct parts with better quasistatic (slow-moving) properties than traditionally wrought materials. Such parts have high yield and flow strengths, making them more resilient in extreme conditions.

SMARTS stands apart from most neutron diffractometers in that it can withstand neutron decay and is therefore ideal for testing

continued on page 7

Don Brown's favorite experiment

What: SMARTS was used to monitor the evolution of the thermal intergranular residual stresses (ITRS) in beryllium.

Why: Beryllium has a hexagonal crystal structure with an anisotropic thermal expansion; the thermal expansion in the *a*-directions are 25% larger than the *c*-direction. In other words, on cooling from the hot-pressing temperature of 1000 ºC, the misfit strain between neighboring grains can be as much as 0.3 %, well beyond the limit of elastic deformation. This results in large residual stresses on the grain (meso-) scale, which can drive dimensional instability in components that can tolerate it, such as mirrors on satellites.

Who: The measurements were completed by Don Brown, Bjorn Clausen, and Thomas Sisneros (MST-8) in collaboration with several other Los Alamos scientists and published in 2009[1].

How: The lattice parameter of beryllium was measured in a solid sample (in which the grains constrain each other) and in a fine powder (in which the grains were not constrained). The difference in the measured lattice parameters was used to determine the ITRS in the solid material. The team is working on repeating these measurements in uranium, which is far more anisotropic. However, uranium powder is very unstable in air, so the powder will be created in situ by a series of hydriding/de-hydriding cycles of the solid sample.

[1] D.W. Brown, T.A. Sisneros, B. Clausen, S. Abeln, M.A.M. Bourke, B.G. Smith, M.L. Steinzig, C.N. Tome, S.C. Vogel, *Acta Mater.*, **57** (2009) 972-979.

Revolutionizing materials for the future with a dynamic mesoscale materials science capability

Materials designed and tailored to perform a specific function are a prime example of science, technology, and engineering innovation that will lead to a revolutionary advance for humanity. With these materials of the future we will be able to design and 3D print materials that are lighter yet stronger or that have better corrosion resistance or discover innovative metamaterials that combine thermal conductivity and electronic properties in unique ways.

Cris Barnes

During a recent Physics and Theoretical Colloquium, I outlined the current vision and status of what the Laboratory is planning as a key piece of a great scientific future for the nation—one that explores the emergent scientific frontier between the atomic and continuum scales for materials in extremes. This middle scale in space and time, the mesoscale, is where atomic and nanoscale systems grow in complexity from emergent behavior at multiple scales and where important properties for continuum system modeling are determined by microstructure and processing variations.

The Department of Energy has recognized this unmet national scientific need, approving a dynamic mesoscale materials science capability (DMMSC) for Critical Decision-0 (mission need) in 2016. Research enabled by this capability supports the strategic and vital goal of production science. Since achievement of CD-0, the technical and program requirements for a DMMSC project have been formally validated by NNSA Defense Programs. Production and infrastructure investments urgently needed by the national enterprise have caused a deferral of progress on this and other scientific capability investments by NNSA. Meanwhile, it is a growing priority of the new LANL Agenda for "Excellence in Mission-Focused STE" to grow LANL's mesoscale science program.

"The broad photon energy range available (from the far IR to hard x-ray) and the intense brightness of the beams, which allows the photon beams to be tailored to specific experimental geometries and environments, makes x-ray light sources near-ideal probes of the structure and function of materials…. As the field moves toward the capability to fully integrate computational materials science, synthesis, and advanced manufacturing for real-world performance, the microscopic characterization of structure and dynamics enabled by the next generation of instruments and upgraded sources will provide the crucial link to enable materials by design."

National Academies Decadal Report on the Frontiers of Materials Research, 2019

"In a data-democratic, technologically-flatter world, the seamless and agile integration from science, technology, and engineering innovation to societal impact will be a differentiator for economic and social prosperity."

Laboratory's Chief Scientist Alan Bishop

To see with time dependence into and through the mesoscale requires x-rays that are coherent, brilliant, and high-repetition rate and of sufficient high energy to probe all strategic materials of interest. The capability also needs multiple different probes at multiple time and length scales to constrain the multiscale science.

The Matter-Radiation Interactions in Extremes (MaRIE) facility, the Laboratory's proposal for studying dynamic mesoscale materials science, is one solution that meets all the validated DMMSC requirements—and it will be a revolutionary capability! MaRIE is envisioned as a 12-GeV electron linac feeding a 42-keV x-ray free-electron laser with experimental facilities. Such an x-ray light source would have unique complementary characteristics to any other facility in the world, including:

- higher x-ray energy for mesoscale systems and high-Z materials;
- higher pulse repetition rate to make movies of microstructure evolution; and
- multiple probes to support maximum science return.

MaRIE would be designed to study materials behavior over an extremely wide range of time scales. We need to understand mesoscale materials from time scales of electronic and ion motion (trillions of times a second) to shock and sound waves (millions of times a second) to thermal times scales of production and manufacturing. That's the "dynamic" part of the project. And the unique highest-energy x-ray laser is needed both to penetrate mesoscale samples and also not heat and destroy the sample despite its brilliance, allowing movies of material behavior. It is being designed with strong connection to the needs of scientific predictive capability from theory, modeling, and computation, all while providing comprehensive materials discovery capability to collaborative teams. The vision is to continue to enable science-based qualification and certification, all while leading to the "revolution in manufacturing/production science."

While the MaRIE design would uniquely and fully fill the identified capability gap, there are present facilities where "dynamic" time-dependent science or "mesoscale" research with higher energy photons can be done. LANL leadership intends to grow our efforts in building capability and delivering results in support of our current mission programs.

I think this is an exciting venture, and I hope many of you will join me!

Cris Barnes, MaRIE Capture Manager

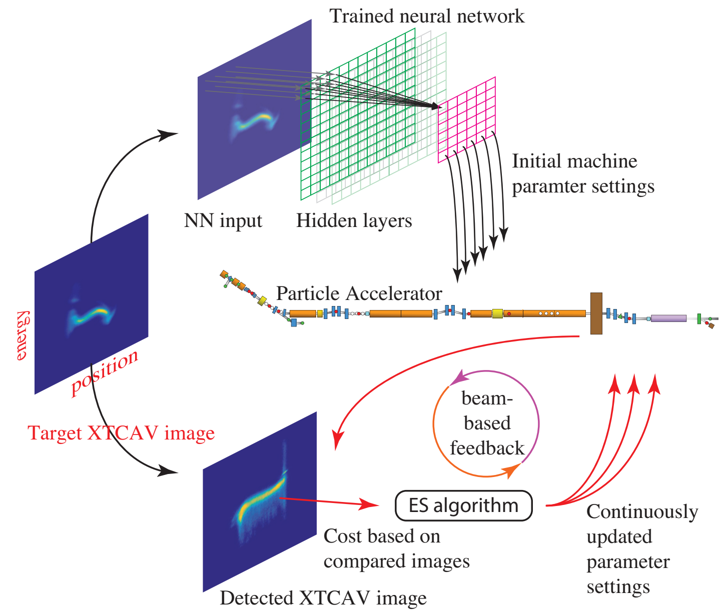
Adaptive feedback automatically tunes electron beams in advanced x-ray free-electron lasers

Next-generation particle accelerators, such as the Linac Coherent Light Source (LCLS) at the SLAC National Accelerator Laboratory and future instruments such as the proposed MaRIE (Matter-Radiation Interactions at Extremes) x-ray free-electron laser (XFEL) at Los Alamos, support NNSA missions. Due to the complexity and uncertainty inherent in their beam generation, quickly and precisely tuning the sophisticated parameters required to accommodate various experimental setups is challenging. This causes valuable beam time lost between setups.

To mitigate this, a team led by Alexander Scheinker (Radio Frequency Engineering, AOT-RFE) with collaborators from SLAC National Accelerator Laboratory is developing a novel hybrid tuning technique to combine machine learning and adaptive feedback to enable fast, automated optical tuning of the particle beams and optimized beam maintenance over time. The team combined a neural network with adaptive feedback to achieve performance beyond what either method could reach on its own. The team demonstrated proof-of-principle of this technique at the LCLS, training a neural network to map 2D longitudinal phase-space distributions of the electron beam. The neural network quickly searched for the desired phase space distribution and then used feedback to determine the correct settings for two different parameters. This network also tracked the correct settings as the accelerator varied over time.

For this initial study, the team focused on just two parameters of the LCLS, which control how much the electron beam is compressed. The researchers performed a 2D grid scan of the parameters and saved a 2D longitudinal phase space distribution at each point. The investigators used the data to train a neural network to predict parameter settings based on 2D phase space distributions. They created a target phase space distribution (not part of the training data) by making large changes in parameter settings. The team used the neural network to predict what the machine parameter settings should be to achieve this target. Because the network must interpolate between training points and the machine characteristics drift with time, the predicted parameter settings resulted in a distribution close to the target but not an exact match. The researchers used model-independent feedback, which completed the tuning by zooming in on the actual correct parameter settings and continuously tracking them as they varied with time. In this demonstration, the target phase space was so dramatically different from the initial machine setup that local model-independent feedback alone became trapped in a local minimum, unable to converge to the correct settings. The team intends to create non-invasive diagnostics that account for the 6 dimensions of phase space and plans to apply the algorithm to tune about 20 parameters at once.

The core algorithm will benefit all particle accelerators, including the linear accelerator at the Los Alamos Neutron



An illustration of the neural network that provided proof-of-principle for the technique. This network was designed to map 2D longitudinal phase space distributions of the LCLS electron beam to LCLS parameter settings. Acronyms: XTCAV = x-band radio frequency transverse deflecting cavity, NN = neural network, ES = extremum seeking.

Science Center. The types of algorithm being developed would especially benefit the Lab's proposed MaRIE XFEL for exploring matter-radiation interactions in extremes. Because MaRIE would be designed to produce extremely closely spaced electron bunches, it would face greater tuning, control, and optimization challenges than existing accelerators.

The work supports the Laboratory's Nuclear Deterrence mission area and its Nuclear and Particle Futures science pillar, especially its accelerators and electrodynamics thrust area.

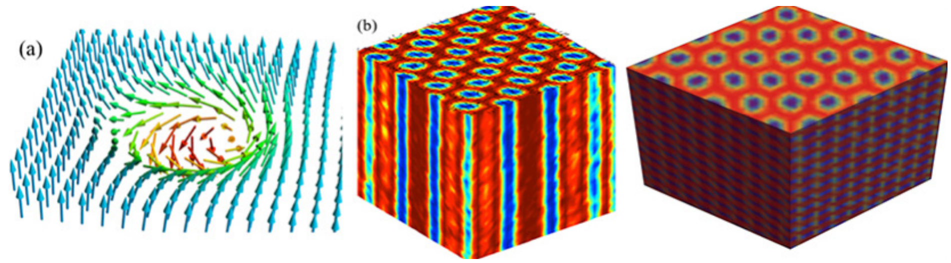
Reference: "Demonstration of model-independent control of the longitudinal phase space of electron beams in the Linac Coherent Light Source with femtosecond resolution," *Physical Review Letters*, 121 (2018). Researchers: Alexander Scheinker (Radio Frequency Engineering, AOT-RFE), Auralee Edelen, Dorian Bohler, Claudio Emma, and Alberto Lutman (SLAC National Accelerator Laboratory).

The Laboratory Directed Research and Development Program funded the work at Los Alamos through its 2018 Momentum Initiative, which aimed to advance two capability thrusts: accelerator capability enhancement and development of advanced accelerators and exploration of mesoscale materials phenomena using state-of-the-art light source user facilities.

Technical contact: Alexander Scheinker

Stabilizing 3D skyrmion crystals

Skyrmions are disk-like objects that typically form triangular crystals in 2D systems. Shi-Zeng Lin and Cristian Batista (Physics of Condensed Matter and Complex Systems, T-4) have demonstrated that different 3D skyrmion crystals can be stabilized in centrosymmetric magnets by tuning the ratio between competing interlayer exchange interactions. *Physical Review Letters* published the research.



(a) Spin profile at the cross section of a skyrmion line. (b) Triangular skyrmion line lattice. (c) Face-centered cubic skyrmion crystal corresponding to the ABCABC stacking of pancake skyrmions in different layers. Color represents the magnitude of the magnetization along the magnetic field direction.

Ions or atoms condense into crystal with various symmetries, depending on the interacting force among them. For instance, salt is made of sodium and chloride, which form a face-centered cubic lattice at room temperature. In magnetic materials, the magnetic polarization can organize into a particle-like texture in the mesoscale. An example is the swirling skyrmion spin texture, which former Los Alamos scientist Tony Skyrme predicted. The swirling skyrmion spin texture has been observed recently in magnets without an inversion center (image “a” in the figure). The skyrmion is regarded as a particle-like excitation because the associated spin texture is well localized in space with a well-defined characteristic size. The size of a skyrmion typically ranges from a few nanometers to hundreds of nanometers depending on the microscopic interactions that stabilize the skyrmions. In bulk crystals skyrmions become line-like objects and crystallize into a triangular line lattice (image “b” in the figure). In thin films the skyrmions are pancake-like objects and form a triangular crystal.

Skyrmions are compact, robust against external perturbations, and can be manipulated by electric currents. Therefore, they could be prime candidates for next-generation spintronic applications such as memory devices. Most skyrmions systems discovered to date do not have an inversion center. According to theory, breaking the inversion symmetry of the crystals is necessary to host the skyrmions. This limits the material choice for skyrmions. Lin and Batista aimed to determine 1) if it is possible to stabilize skyrmion crystals in magnets with inversion symmetry and 2) if skyrmions organize into crystals with symmetries other than the hexagonal symmetry. Their research indicates that both are possible.

In inversion-symmetric rare earth magnets with layered structure, conduction electrons mediate the interaction of localized spins. The interaction is highly oscillatory as a function of the separation between spins. The interaction can be peaked at a nonzero momentum. As a consequence, the ground-state configuration of spins is a helix, where spins rotate along a certain direction. This occurs in many rare earth magnets, such as holmium and erbium. Previous theory predicted that in the presence of a moderate easy axis anisotropy, a triangular lattice of skyrmions could be achieved by applying magnetic field. Because the conditions for stabilizing the skyrmion lattice are general, the skyrmion lattice may exist in the rare earth magnets. The skyrmions in rare earth magnets could have novel properties that do not occur in magnets without an inversion center.

For a ferromagnetic interaction between layers, the skyrmions in each layer stack uniformly along the crystal *c* axis and the magnetic field direction. Therefore, the triangular skyrmion line crystal is stabilized. The researchers investigated the effect of competing magnetic interactions between layers. Generally, the competing interactions introduce modulation in the *c* axis, which tilts the skyrmion lines away from the magnetic field direction. For strong competing interactions, such that the modulation period along the *c* axis is three, which corresponds to the ABCABC… stacking of the pancake skyrmions along the *c* axis, the pancake skyrmions crystallize into a face-centered cubic lattice (image “c” in the figure).

For an antiferromagnetic interlayer coupling, the pancake skyrmions try to avoid piling up uniformly in the *c* axis. This creates an ABAB… stacking of the pancake skyrmions, which corresponds to the hexagonal close-packed lattice. Analogous to real atoms, skyrmions can organize into multiple crystal structures with different responses to external stimuli. This phenomenon makes them suitable for potential technological applications.

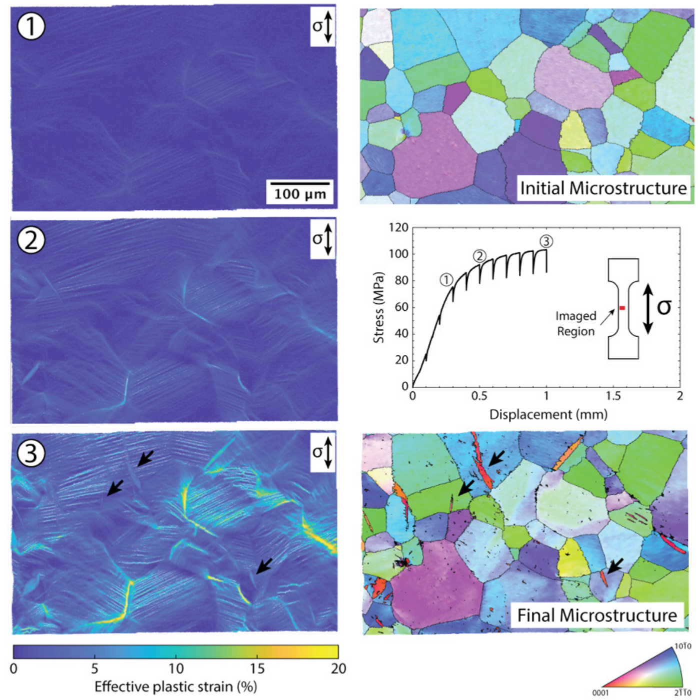
Reference: “Face-centered cubic and hexagonal close-packed skyrmion crystals in centrosymmetric magnets,” *Physical Review Letters* 120, 077201 (2018). Authors: Shi-Zeng Lin and Cristian D. Batista (Physics of Condensed Matter and Complex Systems, T-4).

The Laboratory Directed Research and Development Program funded the work, and the Institutional Computing Program at the Lab provided computer resources for numerical calculations. The research supports the Lab’s Energy Security mission area and the Materials for the Future science pillar through the development of materials for spintronic applications.

Technical contact: Shi-Zeng Lin

New high-resolution strain mapping capability furthers mesoscale materials science

An improved understanding of localized plastic deformation is essential to predicting how a material will respond—and ultimately fail—under extreme conditions. Localized deformation can occur at the mesoscale within individual grains (crystals) due to the physical mechanisms of dislocation slip and twinning, at the micro scale for samples containing multiple grains or phases with differing mechanical properties, or at the continuum level in the case of buckling or shear localization. That the macroscopic plastic deformation of a material can ever be approximated as uniform is the remarkable effect of averaging heterogenous deformations across many length scales. Yet often, and particularly for the damage nucleation and accumulation processes that lead to material failure, grain-level strain localization must be considered explicitly to understand bulk material deformation behavior.



A series of high-resolution local strain maps (left) show how the grain-level processes of slip and twinning transform the initial titanium microstructure (upper right) into the final deformed microstructure (lower right). Data is collected at various times during the tensile test, corresponding to the load drops in the stress-displacement curve (middle right). The field of view is 350 x 550 microns.

To better understand how the mechanical response of a material arises from the complex interactions of localized deformation at the mesoscale, Materials Science in Radiation and Dynamics Extremes (MST-8) researchers have developed for LANL a capability combining in situ digital image correlation (DIC) and scanning electron microscopy (SEM). This technique enables strain to be quantitatively mapped at or below the mesoscale.

When combined with crystal orientation mapping using electron backscatter diffraction (EBSD) and in situ mechanical testing, this technique produces rich data sets containing information about how, when, and to what extent local microscopic plasticity processes contribute to the macroscopic mechanical response and/or failure of a material.

An example of such data is shown in the figure, where high-purity titanium was deformed in tension while capturing high-resolution images for DIC using the Electron Microscopy Laboratory's FEI Apreo SEM. The 350 x 550 micron field of view consists of multiple anisotropic titanium grains in which the strains associated with both slip and twinning are mapped with a spatial resolution below two microns.

Correlation of the strain fields with pre- and post-test EBSD analysis indicates that the primary deformation mechanism is prismatic slip, with some local deformation accommodated by {10-12} and {11-22} twinning. Additionally, the maps reveal high levels of local strain occurring in the vicinity of boundaries between grains with unfavorable orientation relationships for slip transfer. Determining how the local environment of a grain affects the active deformation mechanisms is critical to improving our understanding of how microstructure influences material properties and performance.

Future studies are envisioned that will capitalize on the high spatial strain resolution possible with this technique (spatial resolutions < 100 nm). Example applications include mapping microscale deformation and damage mechanisms in other low symmetry metals and measuring local strains in microstructurally heterogenous or granular composite materials.

Datasets obtained using this technique can guide and complement future experiments at MaRIE, the Laboratory's proposed capability for studying matter-radiation interactions in extremes. MaRIE could allow these types of strain measurements to be extended from 2D to 3D and from quasistatic to dynamic strain rates, further expanding understanding of deformation at the mesoscale.

The development of LANL's SEM-DIC capability for probing the mesoscale response of materials was conducted by Rodney McCabe and Thomas Nizolek (both MST-8).

The work supports the Laboratory's Stockpile Stewardship mission and Materials for the Future science pillar. Funding for the effort was provided through the Institute for Materials Science Rapid Response program and NNSA Science Campaign 2 (LANL Program Manager Dana Dattelbaum).

Technical contacts: Rodney McCabe and Thomas Nizolek

Spotlight on people

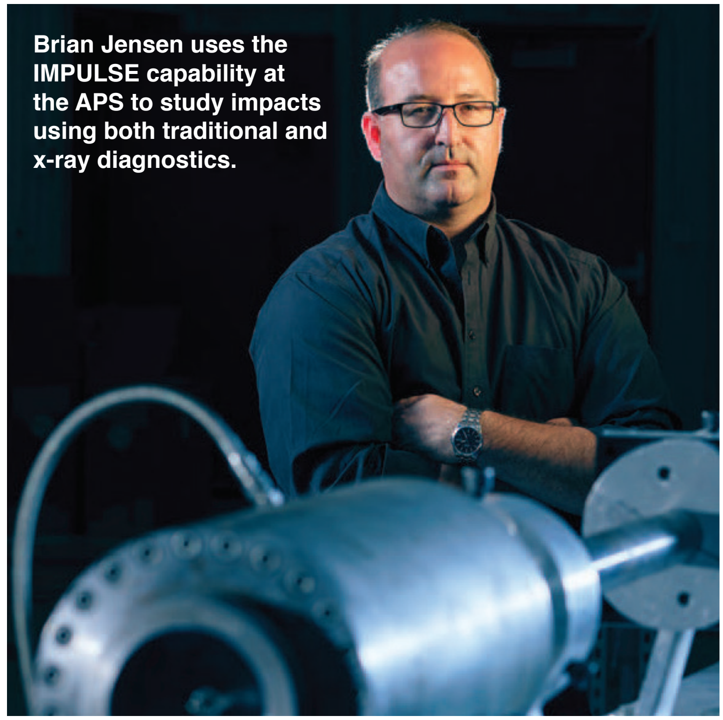
Shock compression researcher Brian Jensen named APS Fellow

Brian J. Jensen (Shock and Detonation Physics, M-9) has been named a 2018 Fellow of The American Physical Society (APS). The APS Shock Compression of Condensed Matter topical group nominated him for "technical leadership in the physics of materials at high pressures, for technical advances in dynamic x-ray diffraction and phase contrast imaging, and for sustained leadership and service to the American Physical Society and the shock physics community."

Jensen's areas of research are x-ray diffraction and phase contrast imaging under shock loading conditions; dynamic, multiphase equations of state for metals, including phase transitions, melting, and temperature measurements; and dynamic experimental facility and advanced diagnostic development.

Jensen, who has a Ph.D. in physics from Washington State University and who joined the Lab in 2004, has received five NNSA Defense Programs Awards of Excellence and is the Lab's point of contact for the Dynamic Compression Sector at Argonne National Laboratory. He led the development of the IMPULSE capability, the first routinely operating impact system at the APS that couples a gun system with a synchrotron beam. It was on this platform that Los Alamos's novel multi-frame x-ray phase contrast imaging system was developed, enabling a new paradigm of experimental research at the APS.

Also named APS Fellows from Los Alamos were Brian Albright (XTD Primary Physics, XTD-PRI), Jennifer Hollingsworth (Center for Integrated Nanotechnologies, MPA-CINT), and Brian Kendrick (Physics and Chemistry of Materials, T-1). The APS is a nonprofit membership organization working to advance and disseminate the knowledge of physics through its research journals; scientific meetings; and education, outreach, advocacy, and international activities. APS represents more than 53,000 members, including physicists in academia, national laboratories, and industry around the world.



Brian Jensen uses the IMPULSE capability at the APS to study impacts using both traditional and x-ray diagnostics.

Technical contact: Brian Jensen

Brown cont.

irradiated materials. However, Brown can't get a full picture of a material with SMARTS alone. He also performs research at high-brilliance, mesoscale-capable imaging facilities such as the Advanced Photon Source at Argonne National Laboratory. There, he tests and refines nonradioactive materials at faster speeds and with better spatial resolution than SMARTS can provide.

Los Alamos's proposed next-level solution for designing and testing materials for the nation's future security needs is MaRIE (for Matter-Radiation Interactions in Extremes). By imaging materials at the mesoscale and in higher resolution than ever before, MaRIE would propel scientists into a new research era beyond the tradition of interring a material's behavior by observing it. MaRIE would have instruments that operate nine orders of magnitude faster than SMARTS, meaning experiments that usually take minutes to resolve would instead take a millionth of a second. A super-hard x-ray free-electron laser would reveal the properties of materials and show them changing in real time. These cutting-edge tools would explain, in unprecedented detail, how materials change under extreme conditions. The end result? Materials designed to have tailored properties and predictable performance.

"MaRIE would provide smaller timescales, improved imaging quality, and compatibility with radioactive or classified parts," said Brown. "The implications for the stockpile are huge."